

Wave functions of the super Tonks-Girardeau gas and the trapped 1D hard sphere Bose gas

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Recent theoretical and experimental results demonstrate a close connection between the super Tonks-Girardeau (sTG) gas and a 1D hard sphere Bose (HSB) gas with hard sphere diameter nearly equal to the 1D scattering length a_{1D} of the sTG gas, a highly excited gas-like state with nodes only at interparticle separations $|x_{j\ell}| = x_{\text{node}} \approx a_{1D}$. It is shown herein that when the coupling constant g_B in the Lieb-Liniger interaction $g_B\delta(x_{j\ell})$ is negative and $|x_{12}| \geq x_{\text{node}}$, the sTG and HSB wave functions for $N = 2$ particles are not merely similar, but identical; the only difference between the sTG and HSB wave functions is that the sTG wave function allows a small penetration into the region $|x_{12}| < x_{\text{node}}$, whereas for a HSB gas with hard sphere diameter $a_{\text{h.s.}} = x_{\text{node}}$, the HSB wave function vanishes when $|x_{12}| < a_{\text{h.s.}}$. Arguments are given suggesting that the same theorem holds also for $N > 2$. The sTG and HSB wave functions for $N = 2$ are given exactly in terms of a parabolic cylinder function, and for $N \geq 2$, x_{node} is given accurately by a simple parabola. The metastability of the sTG phase generated by a sudden change of the coupling constant from large positive to large negative values is explained in terms of the very small overlap between the ground state of the Tonks-Girardeau gas and collapsed cluster states.

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If an ultracold atomic vapor is confined in a de Broglie wave guide with transverse trapping so tight and temperature so low that the transverse vibrational excitation quantum is larger than available longitudinal zero point and thermal energies, the effective dynamics becomes one-dimensional (1D) [1, 2]. 3D Feshbach resonances [3] allow tuning to the neighborhood of 1D confinement-induced resonances (CIRs) [1, 4], where the 1D interaction is very strong, leading to strong short-range correlations, breakdown of effective-field theories, and emergence of highly-correlated N -body ground states. In the bosonic case with zero-range repulsion $g_B\delta(x_j - x_\ell)$ with coupling constant $g_B \rightarrow +\infty$, the Tonks-Girardeau (TG) gas, the exact N -body ground state was determined in 1960 by a Fermi-Bose (FB) mapping to an ideal Fermi gas [5], leading to “fermionization” of many properties of this Bose system, as recently confirmed experimentally [6, 7]. It is now known [8–10] that the FB mapping is of much greater generality; when supplemented by an inversion and sign change of the coupling constant, it provides a mapping between the N -body energy eigenstates of a 1D Bose gas with delta-function interactions $g_B\delta(x_j - x_\ell)$ of any strength [Lieb-Liniger (LL) gas [11]] and those of a spin-aligned Fermi gas.

Practically all experiments on ultracold Bose gases with tight transverse trapping (1D regime) are for the case where, in addition to tight transverse trapping, there is weak longitudinal trapping by a harmonic oscillator potential $m\omega^2 x^2/2$ where x is the longitudinal coordinate. In that case the strength of effective 1D LL boson-boson interactions is characterized by a dimensionless coupling constant $\lambda = g_B/2^{3/2}\hbar\omega x_{\text{osc}}$ where $x_{\text{osc}} = \sqrt{\hbar/m\omega}$ is the

oscillator length. For $\lambda \rightarrow +\infty$ the exact ground state is the trapped TG gas, and for $\lambda \rightarrow -\infty$ the same TG state is still an exact eigenstate (though now highly excited), since both cases map to the ideal Fermi gas [5, 8]. If λ is negative and finite, the ground state is very different; it is McGuire’s collapsed cluster state (bright soliton) [13]. However, if λ is very large and negative, it was first shown theoretically [14–16] that the system is metastable against collapse to McGuire’s cluster state in spite of the very strong attractive interactions, and exhibits a strong similarity with a trapped 1D hard sphere Bose (HSB) gas with hard sphere diameter $a_{\text{h.s.}} > 0$ nearly equal to the 1D scattering length a_{1D} of the system with $\lambda < 0$. It is even more highly correlated than the TG gas, and hence was named [14] the “super Tonks-Girardeau” (sTG) gas. By changing λ suddenly from large positive to large negative values by passing through the CIR, the sTG gas was recently created experimentally and shown to have properties in agreement with the theoretical predictions [17].

Exact solution for $N = 2$: In the simplest case of two bosons with LL interaction $g_B\delta(x_1 - x_2)$ in a harmonic trap potential $m\omega^2(x_1^2 + x_2^2)/2$, all energy eigenstates and eigenvalues can be easily obtained. The wave function for the center of mass (c.m.) coordinate $X = (x_1 + x_2)/2$ is $\psi_{\text{c.m.}} = \exp[-X^2/x_{\text{osc}}^2]$ and its energy is $E_{\text{c.m.}} = \hbar\omega/2$ assuming that the c.m. mode is unexcited. Denote the relative wave function by $\phi(x)$ with $x = x_1 - x_2$. The excited eigenstates $\psi_\nu(x_1, x_2)$ are most easily found by FB mapping [5]. The Fermi-Bose (FB) mapping relation [5] reduces to $\phi_B(x) = -\text{sgn}(x)\phi_F(x)$. ϕ_B satisfies the same harmonic oscillator (HO) wave equation as ϕ_F for

$x \neq 0$, and at $x = 0$ both satisfy a derivative condition which for ϕ_F reads

$$\phi_F'(0\pm) = (\mu g_B/\hbar^2)\phi_F(0+) = -(\mu g_B/\hbar^2)\phi_F(0-) \quad (1)$$

where μ is the effective mass $m/2$. Since ϕ_F is fermionic, it is an odd function, but nevertheless it does not vanish at $x = 0$; instead, it changes sign there, but its derivative is continuous. For $x \neq 0$, ϕ_F satisfies the free particle HO wave equation valid for $x \neq 0$ supplemented by the cusp boundary condition (1). Two different solutions of the HO wave equation having nonzero value and nonzero derivative at $x = 0$ are required, such that the boundary conditions of (1) are satisfied. These cannot be satisfied by the usual Hermite-Gaussian solutions; instead, solutions which are essentially analytic continuations of these to nonintegral quantum number n are required. Since ϕ_F is necessarily an odd function of x , it is sufficient to obtain a solution y of the differential equation only for $x > 0$, taking $\phi_F(x) = y(q)$ for $x > 0$ and $\phi_F(x) = -y(|q|)$ for $x < 0$, where $x = qx_{\text{osc}}$. The necessary solution vanishing and integrable as $q \rightarrow +\infty$ is a parabolic cylinder function $D_\nu(q)$ expressible in terms of confluent hypergeometric series $\Phi(\alpha, \gamma; z)$ which is a sum of two terms, one even and the other odd in q [18–22].

$$D_\nu(q) = 2^{\frac{\nu}{2}} e^{-\frac{q^2}{4}} \left[\frac{\sqrt{\pi}}{\Gamma(\frac{1}{2} - \frac{1}{2}\nu)} \Phi\left(-\frac{\nu}{2}, \frac{1}{2}; \frac{q^2}{2}\right) - \frac{q\sqrt{2\pi}}{\Gamma(-\frac{\nu}{2})} \Phi\left(\frac{1}{2} - \frac{1}{2}\nu, \frac{3}{2}; \frac{q^2}{2}\right) \right]. \quad (2)$$

This solution vanishes like $q^\nu e^{-q^2/4}$ as $q \rightarrow +\infty$; it diverges like $|q|^{-\nu-1} e^{q^2/4}$ as $q \rightarrow -\infty$, but that is of no consequence since we require it only for $q > 0$. The relative energy eigenvalues are $E_{\text{rel}} = (\nu + \frac{1}{2})\hbar\omega$ where the nonintegral quantum numbers ν are determined by the derivative condition (1). This leads to the following transcendental equation for the allowed values [21]: $\Gamma(\frac{1}{2} - \frac{1}{2}\nu)/\Gamma(-\frac{1}{2}\nu) = -\lambda$ in terms of the previously defined dimensionless coupling constant λ . Multiplying by the signum function so as to obtain the bosonic (even) solution $\phi_B(x) = -\text{sgn}(x)\phi_F(x)$ one obtains a bosonic solution continuous and nonzero at $x = 0$ but with a cusp (derivative sign change) there. The total wave function including the c.m. factor can be written as $\psi_{B\nu}(x_1, x_2) = \exp[-(x_1^2 + x_2^2)/2x_{\text{osc}}^2] f_\nu(|q|)$ where $f_\nu(|q|) = D_\nu(|q|) e^{q^2/4}$ and $q = (x_1 - x_2)/x_{\text{osc}}$. The exponential growth of $e^{q^2/4}$ as $|q| \rightarrow \infty$ is cancelled by the exponential decrease of $D_\nu(|q|)$ like $e^{-q^2/4}$.

The first excited state is the one with $\nu \rightarrow 1$ as $|\lambda| \rightarrow \infty$ and has only one node at $|x_1 - x_2| = x_{\text{node}}$. For $|\lambda| = \infty$, ϕ_F is just the first excited HO state $qe^{-q^2/2}$ [12] with a node only at the origin, and for finite negative λ , $x_{\text{node}} > 0$. It is clear from Figs. 5(b,c,d) of [21] that ϕ_B is almost linear in the region $0 \leq |x| \leq x_{\text{node}}$ for all negative

λ , so it is well approximated there by a parabola, which can be found explicitly from the leading terms of the hypergeometric series in Eq. (2) and the Gaussian prefactor. By Eq. (2), [18], and the transcendental equation for ν one finds $\phi_B \approx c\{|q| - \frac{a_{1D}}{x_{\text{osc}}}[1 - (\frac{\nu}{2} + \frac{1}{4})q^2] + \dots\}$ where c is a normalization constant. The node is then at $x_{\text{node}} = a_{1D}[1 - (\frac{\nu}{2} + \frac{1}{4})(\frac{a_{1D}}{x_{\text{osc}}})^2] + \dots$, which is very close to a_{1D} when $a_{1D} \ll x_{\text{osc}}$, the case when $|\lambda| = x_{\text{osc}}/\sqrt{2}a_{1D} \gg 1$.

The ground state is very different from the excited states, being a collapsed state which is an analog, for the trapped system, of McGuire's cluster state [13]. It is an even solution also expressible in terms of a D_ν , but one whose energy approaches $-\infty$ as $g_B \rightarrow -\infty$ ($a_{1D} \rightarrow 0+$); see Fig. 5 of [21]. For $a_{1D} \rightarrow 0+$ it is well approximated by $\psi_{B0} \approx \exp(-|x_1 - x_2|/a_{1D}) \exp[-(x_1^2 + x_2^2)/2x_{\text{osc}}^2]$; in fact, this expression satisfies the $x_{12} \rightarrow 0$ contact condition exactly and becomes exact for all (x_1, x_2) in both limits $a_{1D} \rightarrow 0+$ (total collapse) and $a_{1D} \rightarrow +\infty$ (ideal Bose gas).

Comparison with trapped hard sphere gas: The recent theoretical [14–16] and experimental [17] results demonstrate a close connection between the sTG gas and a 1D hard sphere Bose (HSB) gas with hard sphere diameter $a_{\text{h.s.}}$ nearly equal to a_{1D} , the 1D scattering length of the sTG gas. Actually, when all interparticle separations $|x|$ are larger than the nodal position x_{node} , the sTG and HSB wave functions are not merely similar, but identical, provided that one sets the hard sphere diameter $a_{\text{h.s.}} = x_{\text{node}}$. We prove this first in the simplest case $N = 2$. It is sufficient to restrict ourselves to the region $x \geq x_{\text{node}}$; the solution for $x \leq -x_{\text{node}}$ can then be obtained by replacing the argument x by $|x|$. The parabolic cylinder function D_ν defined by Eq. (2) [18–22] satisfies the correct Schrödinger equation for $x > x_{\text{node}}$ as well as the correct boundary conditions of vanishing at $|x| = x_{\text{node}}$ and infinity and is normalizable, so it is certainly an allowable energy eigenstate for hard spheres of diameter x_{node} . The only remaining question is whether it is the *ground* state for that given hard sphere diameter. Since Schrödinger's equation for the given region and boundary conditions is a well-posed Dirichlet problem and the solution given by D_ν is nodeless in this region, it follows from Sturm-Liouville theory that it is the hard sphere ground state. At $|\lambda| = \infty$, D_ν reduces to the TG ground state [12], which is indeed the ground state for hard spheres of diameter $x_{\text{node}} = 0$ zero. As $|\lambda|$ decreases, this node moves out from the origin, and the solution given by D_ν for $x \geq x_{\text{node}}$ continues to be the ground state for $|\lambda| < \infty$. The *only* difference between the sTG and HSB wave functions apart from normalization is that the sTG wave function allows penetration into the region $|x| < a_{\text{h.s.}}$. This holds for $-\infty < \lambda < 0$, and the penetration is small when $|\lambda| \gg 1$ so that $x_{\text{node}} = a_{\text{h.s.}} \approx a_{1D}$. Furthermore, the sTG and hard sphere solutions have the same energy. We emphasize that when the wave function

is extended into the interior region $|x| < x_{\text{node}}$ the resultant sTG wave function is highly excited relative to the collapsed McGuire state due to the effects of the strong attraction at $x = 0$, but when restricted to the region $|x| \geq x_{\text{node}}$, it is *identical* with the *ground* state of the hard sphere Bose gas apart from normalization, and the energies of the *highly excited* sTG state and the hard sphere *ground* state are exactly equal [24].

Generalization to $N > 2$: The ground state in the (x_1, \dots, x_N) space including the interaction points $x_j = x_\ell$ is the trapped version of McGuire's cluster state, and one expects that for $a_{1D} \rightarrow 0+$ it will be well approximated by

$$\psi_{B0} \approx \left[\prod_{1 \leq j < \ell \leq N} \exp\left(-\frac{|x_j - x_\ell|}{a_{1D}}\right) \right] \prod_{j=1}^N \exp\left(-\frac{x_j^2}{2x_{\text{osc}}^2}\right). \quad (3)$$

In fact, the LL contact conditions [11] arising from the delta interactions $g_B \delta(x_j - x_\ell)$ are satisfied exactly at each collision point $x_j = x_\ell$. Furthermore, this expression becomes exact at all (x_1, \dots, x_N) in both limits $a_{1D} \rightarrow 0+$ (total collapse) and $a_{1D} \rightarrow \infty$ (trapped ideal Bose gas), as well as when $x_{\text{osc}} \rightarrow \infty$. In view of the ubiquity of such Bijl-Jastrow pair product wave functions as exact energy eigenstates of 1D Bose and Fermi gases [5, 10, 12, 25–27], we expect that the sTG state will also be well approximated by such a pair product. The obvious generalization of the $N=2$ sTG wave function to arbitrary N is

$$\psi_{B\nu}(x_1, \dots, x_N) = \left[\prod_{1 \leq j < \ell \leq N} f_\nu(|q_{j\ell}|) \right] \prod_{j=1}^N \exp\left(-\frac{x_j^2}{2x_{\text{osc}}^2}\right) \quad (4)$$

where $f_\nu(|q_{j\ell}|) = D_\nu(|q_{j\ell}|) e^{q_{j\ell}^2/4}$ and $q_{j\ell} = (x_j - x_\ell)/x_{\text{osc}}$. It also satisfies the contact conditions exactly, and becomes exact at all (x_1, \dots, x_N) in both limits $a_{1D} \rightarrow 0+$ (trapped TG gas, where $\nu = 1$ and $f_\nu = |q_j - q_\ell|$) and $a_{1D} \rightarrow \infty$ (trapped ideal Bose gas, which maps to the trapped FTG gas [25, 26], and where $\nu = 0$ and $f_\nu = 1$).

There are accurate numerical solutions for $N = 3$ which prove the existence of a gas-like excited state with nodes *only* at a nearest neighbor separation $|x_{j\ell}| = x_{\text{node}}$ which increases with decreasing $|\lambda|$, is very close to a_{1D} for $|\lambda| \gg 1$, and goes to zero along with a_{1D} in the TG limit $|\lambda| \rightarrow \infty$; see Fig. 4 of [22]. Furthermore, for all $N \geq 2$ the approximate wave functions (4) vanish only at $|x_{j\ell}| = x_{\text{node}}$ and become exact both at the collision points $x_{j\ell} = 0$ and when all $|x_{j\ell}| \rightarrow \infty$, and we expect the exact sTG solution to have the same properties. We expect that the theorem on the identity of the sTG and hard sphere wave functions and energies in the region exterior to the nodes will also hold for all $N > 2$ since the exact hard sphere ground state for hard sphere diameter $x_{\text{node}} = 0$ is the $|\lambda| = \infty$ TG ground state [12] and the same arguments we used for $N = 2$ should apply as $|\lambda|$

is decreased. A rigorous appeal to Sturm-Liouville theory would require a proof that for the *exact, unknown* sTG eigenfunctions the pair distribution function vanishes only at $|x_j - x_\ell| = x_{\text{node}}$, and so far this is known only for $N = 2$ and $N = 3$ [22]. Therefore we state our belief of the identity of the sTG and hard sphere wave functions and energies for all N as a conjecture.

Sudden approximation and metastability: In the experiment by the Innsbruck group [17], the dimensionless coupling constant λ is changed suddenly from large positive to large negative values. For $\lambda \gg 1$ the ground state is very close to that of the trapped TG gas, the ground state for $\lambda = +\infty$, whose *exact* wave function is $\psi_{TG} = C_N [\prod_{1 \leq j < \ell \leq N} |x_j - x_\ell|] \prod_{j=1}^N \exp(-x_j^2/2x_{\text{osc}}^2)$ where C_N is a normalization constant [12]. Assuming that the switch to large negative λ is rapid enough that the sudden approximation is valid, the wave function after the switch will be in a superposition of all eigenstates $\psi_{\lambda\alpha}$ of the system with negative λ : $\psi_\lambda(t) = \sum_\alpha \langle \psi_{\lambda\alpha} | \psi_{TG} \rangle \psi_{\lambda\alpha} e^{-iE_{\lambda\alpha}t/\hbar}$. The stability of a trapped gas with attractive 1D interaction was addressed in [17] by measuring the frequencies of collective breathing mode. It was found that by rapidly crossing the CIR to finite positive a_{1D} the frequency increases, which agrees with the description of the sTG state in terms of an equivalent hard rod system, while at larger values of a_{1D} the frequency decreased. These results agree with our theorem that the sTG state has the same ground state energy as a system of hard spheres, increasing with density [28, 29], so that the frequency in the sTG state increases with a_{1D} , although for non-zero values of a_{1D} there is a possibility of populating states different from the sTG state. We analyze the transition through the CIR in terms of the projection of the TG state to the gas-like sTG eigenstate and states that contain bound states, relying on the fact that the initial state for $\lambda \gg 1$ is very close to the $\lambda = +\infty$ TG state. In the above expression for $\psi_\lambda(t)$ there are many-body bound states with $N = 2, \dots, N$ particles, with the bound part described by McGuire's many-body solution Eq. (3) with a characteristic size of a_{1D} . The projection integral $\langle \psi_{\lambda\alpha} | \psi_{TG} \rangle$ decreases exponentially fast with the number of particles in the bound state. From this the most probable way to transfer particles to some bound state is to do so to a bound state with 2 particles. We calculate the projection integral $\langle \psi_{\lambda\alpha} | \psi_{TG} \rangle$ for different numbers of particles and show the results in Fig. 1. The transition to many-particle bound states is highly suppressed compared to the transition to a state where two particles are bound while all the other particles are unbound. This can be understood by comparing characteristic volumes that a state occupies in the phase space. The typical size of a McGuire state of N particles is a_{1D}^N , while the TG gas occupies $(\sqrt{N}x_{\text{osc}})^N$, so that the overlap decreases dramatically as N is increased. From this the most relevant transition is to a state with two particles bound. The

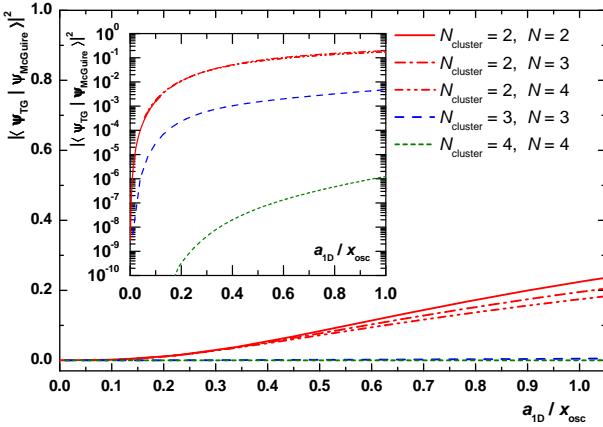


FIG. 1: Square of overlap integral of TG gas-like state with a McGuire state containing N_{cl} clustered particles, as a function of a_{1D}/x_{osc} . Inset, the same data on a semi-logarithmic scale.

overlap integral was evaluated analytically for 2 bound particles in systems of $N = 2, 3, 4$ particles, and numerically for bound clusters of 3 and 4 particles, with the bound cluster described by the McGuire wave function (3) while leaving the other particles in the TG state. In all cases the overlap is very small when $a_{1D} \ll x_{\text{osc}}$, as in the experiment [17].

These results are expected since ψ_{TG} is an exact eigenstate not only for $\lambda = +\infty$, but also for $\lambda = -\infty$, since both map to the ideal Fermi gas [5, 8]. Hence the system is *completely stable* under a sudden jump from $\lambda = +\infty$ to $\lambda = -\infty$, and metastable following a jump from $\lambda \gg 1$ to $\lambda \ll -1$.

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